

## ELECTRONIC AND MOLECULAR STRUCTURE OF CARBON GRAINS\*

Jan Almlöf and Hans-Peter Lüthi

Minnesota Supercomputer Institute

Clusters of carbon atoms have been studied with large-scale *ab initio* calculations. Planar, single-sheet graphite fragments with 6 - 54 atoms were investigated, as well as the spherical C<sub>60</sub> "Buckminsterfullerene" molecule. Polycyclic aromatic hydrocarbons (PAHs) have also been considered. Thermodynamic differences between diamond- and graphite-like grains have been studied in particular. Saturation of the peripheral bonds with hydrogen is found to provide a smooth and uniform convergence of the properties with increasing cluster size. For the graphite-like clusters the convergence to bulk values is much slower than for the three-dimensional complexes.

Introduction.

Due to their scientific and technical importance, carbon clusters have long been subject to a variety of experimental[1-24] and theoretical[25-51] investigations. The areas of interest are of great diversity, including heterogeneous catalysis, the composition of graphite vapor, soot formation during combustion[15] and early stages of synthetic natural gas production from coal. Several small clusters have been identified spectroscopically in the atmospheres of red giant stars and in comet tails[6-9].

The experimental work reported for carbon clusters ranges from the early investigations of Honig and Drowart et al on small clusters[1-3] to the recent studies in the groups of Smalley and Kaldor[10-16] on larger clusters with up to 200 atoms.

A striking observation that lacks a satisfactory explanation is the existence of 'magic numbers', i.e. the fact that in a distribution of clusters some species with a certain number of carbon atoms are much more abundant than others. The exact clustering mechanisms are not completely understood, and, as noted by e.g. Rohlffing et al.[10], the origin of the observed distribution of clusters may depend upon instrumental factors. Accounting for this fact, however, there still seems to be a preference for clusters with certain numbers of atoms which cannot be explained solely as due to the experimental conditions.

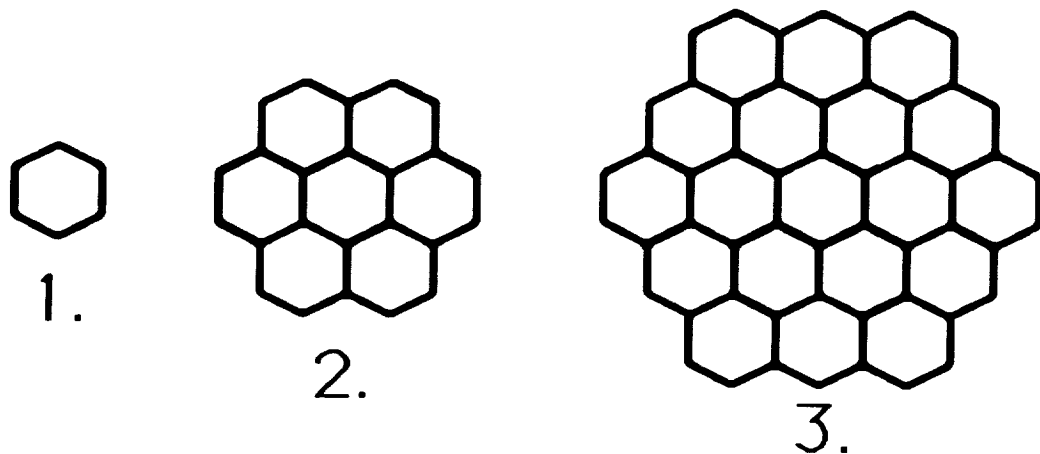
Evidently, several aspects of this exciting area are difficult to study with experimental techniques. The different species are short-lived, reactive, and exist only under rather extreme conditions. These are conditions under which theoretical studies can contribute a lot to our understanding. Theoretical work has indeed been reported on smaller clusters with  $n=2-10$ [42-50] as well as on some of the larger ones[25-41]. The present work reports *ab initio* calculations for a number of large carbon clusters of relevance for the chemical problems addressed above.

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*Ab initio* investigations on systems of the size considered here are usually not considered a routine procedure. Calculations which account for electron correlation in a meaningful fashion are still beyond reach for most of these molecules. With recent progress in hardware and software development it is now technically and economically feasible to study quite large molecules using the Hartree-Fock method. That approach has also the advantage of being size consistent, which is a necessity for this type of study when results for molecules of vastly different size are to be compared. This allows for the selection of study species which may at first be relatively small, but which may be gradually increased to sizes that eventually strain the capacity of the computing equipment. Size-consistency allows for an extrapolation of these results to even larger molecules, eventually to bulk systems, which are far beyond reach for a direct application of these computational methods.

### Graphite-like Fragments

Due to the enormous number of possible structures for all but the few smallest clusters, quite restrictive assumptions about their geometry have to be made. For those clusters where well-defined equilibrium structures do exist, these are likely to possess a non-trivial point group symmetry (in many cases the highest possible symmetry). It therefore seemed justified to focus the study on high-symmetric systems. Symmetry can also be used to simplify the calculation of electronic structure, and reduces the number of geometrical degrees of freedom to be optimized. In order to further confine the study, only graphite-like systems consisting of pericondensed aromatic six-rings are considered.



**Figure 1.** Graphite-like fragments of  $D_{6h}$  symmetry.  $C_6$ (1),  $C_{24}$ (2) and  $C_{54}$ (3).

In an initial series of calculations, the systems  $C_6$ ,  $C_{24}$  and  $C_{54}$  ( $D_{6h}$  symmetry, 1, 2 and 3 in Fig. 1) were computed in a high spin form with all unpaired electrons having parallel spins (Total spin  $S=3, 6$ , and  $9$ ). All carbon-carbon bond distances were kept equal at  $1.42 \text{ \AA}$ , the distance experimentally found in bulk graphite(55). The total energies computed,  $-226.5321$  Hartree for  $C_6$ ,  $-907.0085$  Hartree for  $C_{24}$  and  $-2041.5720$  Hartree for  $C_{54}$ , can be interpreted in terms of cohesive energies of  $71.0$ ,  $97.1$  and  $106.5$  kcal/mol per carbon atom, respectively.

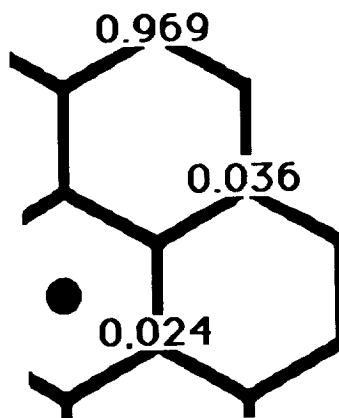
Apparently, the cohesive energy of these clusters shows a very slow convergence with the size of the molecule. This should not be surprising, since the number of unsaturated valences "dangling bonds" per carbon atom is one in 1, one-half in 2 and one-third in 3.

Assuming an approximately constant energy per C-C bond, the above trend is understandable. With clusters on the above general type, the number of carbon atoms is  $6N^2$ , the number of dangling bonds is  $6N$  and the number of C-C bonds is  $9N^2 - 3N$ . The energy per bond shows a smoother trend, the numbers being 71.0, 77.6 and 79.9 kcal/mol, respectively. Alternatively, the energies can be fitted to a two-parameter expression of the form

$$E_{\text{tot}} = 6N^2 E_C + 6NE_{\text{db}} \quad (1)$$

where  $E_C$  (energy per carbon atom) and  $E_{\text{db}}$  (energy per dangling bond) are adjustable parameters. The optimum coefficients are  $E_C = -37.8366$  Hartree and  $E_{\text{db}} = +0.0891$  Hartree. For large values of  $N$  the total energy per carbon atom will converge towards  $E_C$ , and accordingly the cohesive energy of  $N$  the total energy per carbon atom will converge towards  $E_C$ , and accordingly the cohesive energy per carbon atom in graphite can be expressed as the difference between  $E_C$  and the atomic energy of carbon ( $-37.6371$  Hartree), leading to a value of  $0.1995$  Hartree or  $125$  kcal/mol. (i.e.  $83.3$  kcal/mol per C-C bond, since in graphite there are  $3/2$  bonds per carbon atom). The parameter  $E_{\text{db}}$ , for which a value of  $+0.0891$  Hartree is derived, can be interpreted as the energy loss (note the positive sign of  $E_{\text{db}}$ ) for introducing a dangling bond in a graphite-like sheet of carbon atoms. Since breaking a C-C bond would result in two dangling bonds, the value of  $E_{\text{db}}$  corresponds to a loss of bond energy of  $112$  kcal/mol per bond, somewhat higher than the bond energy derived from  $E_C$ . One might have expected the electrons unpaired by the bond-breaking to redistribute into other bonding orbitals, or, in valence-bond language, that the broken peripheral bonds would rehybridize to minimize the destabilization of the framework. The opposite turns out to be true, though; breaking some bonds weakens others due to an interrupted electron delocalization, a phenomenon illustrated by the fact that the C-C bond in cyclic  $C_6$  is considerably weaker than in graphite.

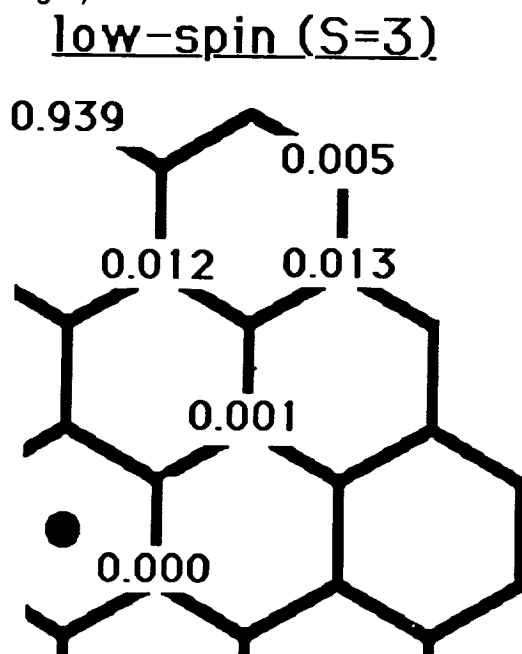
For the larger clusters  $C_{24}$  and  $C_{54}$  all carbon atoms are not symmetry equivalent, and fluctuations in the local properties from atom to atom may occur. It is of some interest to study the details of that fluctuation. For instance, it is important to know how large the molecule needs to be before its interior is reasonably close to that of a single-sheet graphite. The population analysis for  $C_{24}$  shown in Fig. 2 demonstrates that the charge originating from the unpaired electrons is located to a large extent in the peripheral carbon sigma-bonding orbitals.



**Figure 2.** Spin-density populations for  $C_{24}$  in a high-spin form ( $S=6$ ).

So far, only high-spin systems have been considered. However, when neighboring dangling bonds interact, spin-pairing may occur and lead to the formation of new bonds, and hence to a lower

energy. In the case of  $C_{24}$  all adjacent dangling bond electrons can be paired up, which would result in a singlet state of the molecule. A partial structure optimization on this state leads to very short peripheral carbon-carbon bonds (1.20 Å) with essentially triple bond character. All other bond lengths change very little despite the strain introduced by shortening one bond of the outer six-membered ring by more than 0.2 Å. For  $C_{54}$  a similar structure may be obtained. Pairing up electrons from adjacent carbon atoms of the same six-membered ring, and leaving all the other (isolated) dangling bond electrons with parallel spins, a low spin state ( $S=3$ ) would be obtained. This mechanism is supported by an actual calculation on the low spin form, in which the spin density is almost entirely localized on the carbon atom that would carry the dangling bond in a simple valence orbital picture. (see Fig 3).



**Figure 3.** Spin density distribution for  $C_{54}$  in a low-spin form ( $S=3$ ).

Energy calculations show that the low spin state of  $C_{54}$  is indeed about 1.3 eV lower in energy than the high spin state, at least for the molecular geometries used here, whereas for  $C_{24}$  nearly identical energies for the two states are found. Inclusion of electron correlation would favor the low spin form further, though hardly enough to significantly affect a comparison of cohesive energies between various forms of carbon.

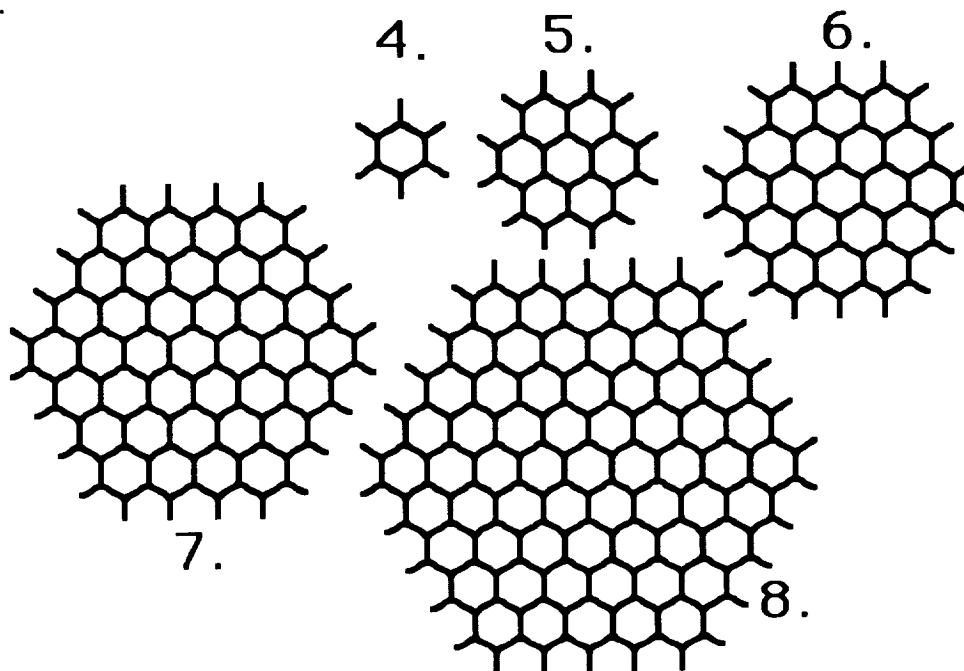
The ionization potentials (Koopmans' values) for the high spin and the low spin form of  $C_{54}$  are 6.8 and 7.3 eV respectively, values that would both fit into the bracket of IP's reported for carbon clusters with 40 to 100 atoms[11]. The corresponding values for  $C_{24}$  are higher, 8.0 and 8.3 eV respectively.

### Polycyclic Aromatic Hydrocarbons.

The above studies show that properties in the interior of the graphite-like clusters do not converge readily to bulk values. Even for the  $C_{54}$  cluster, the populations in the center show a significant deviation from neutrality. Despite the possibility of exploiting the high point-group symmetry of these systems, the complicated open-shell structure places severe limits on the maximum

size of the clusters that can be studied. Therefore, the calculation of a graphite cluster large enough to ensure that the calculated properties have converged to bulk values would be computationally unfeasible.

If the focus of interest is on the carbon clusters themselves, then of course no substitute system can be used. However, for studying the convergence of properties one can minimize the termination effects by saturating the dangling bonds in the simplest possible way, i.e. with hydrogen. By that approach one can both avoid the problem of handling an excessive number of open shells, and obtain a series of molecules that converge towards bulk properties more smoothly than the bare carbon clusters.



**Figure 4.** The PAHs  $C_6H_6$ (4),  $C_{24}H_{12}$ (5),  $C_{54}H_{18}$ (6),  $C_{96}H_{24}$ (7), and  $C_{150}H_{30}$ (8)

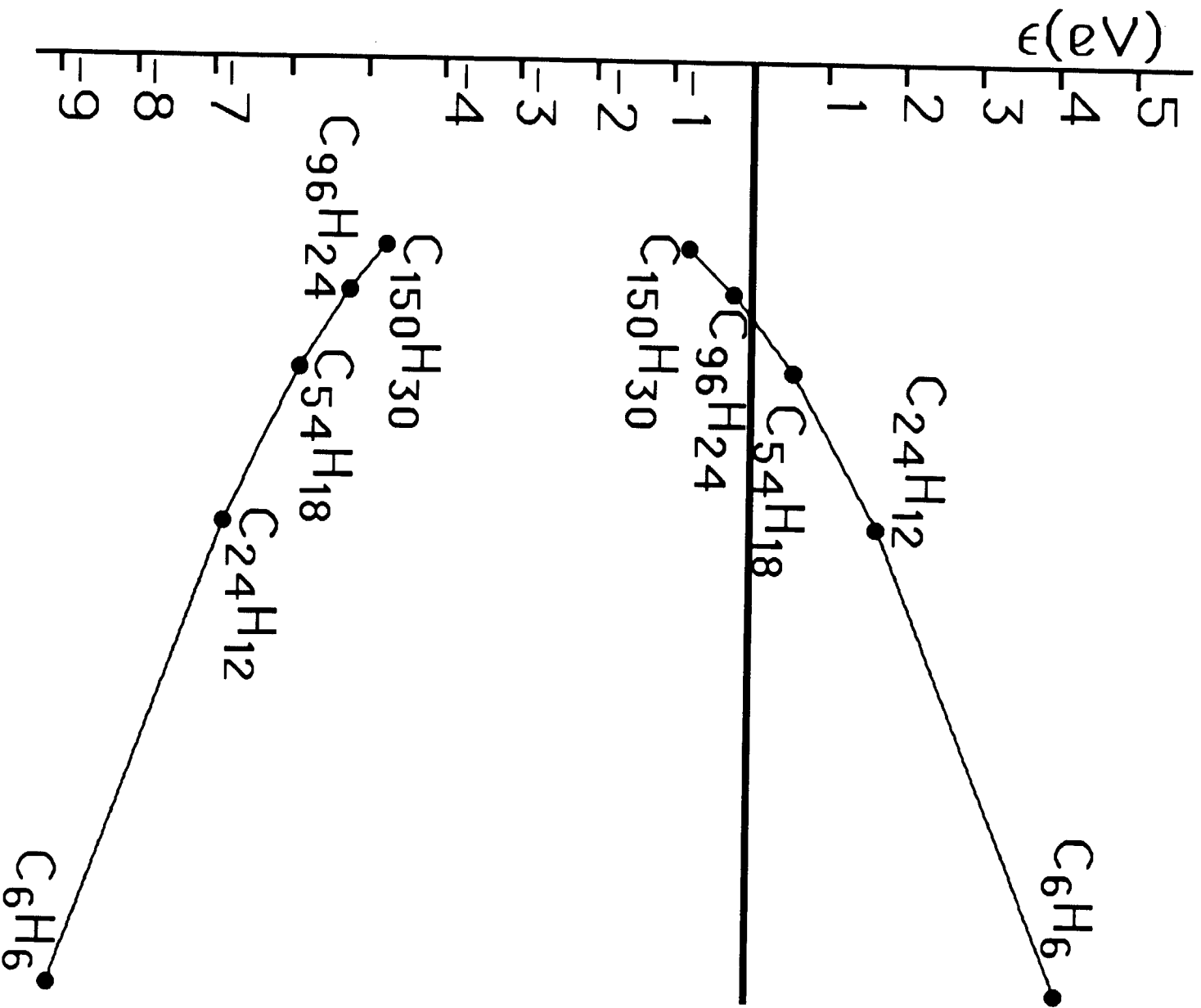
The series of PAHs shown in Fig. 4 have been studied in the present work, and should allow for an extrapolation towards an infinite single layer of graphite. The total energies of these systems with the general formula  $C_{6N}H_{6N}$  are presented in Table 1. For all molecules except 8 an overall C-C bond distance was optimized. This seems to converge smoothly towards 1.406 Å, a value somewhat shorter than that experimental distance of 1.421 Å found in bulk graphite[52]. The Hartree-Fock approximation is the main source of this discrepancy. It should be noted, however, that the bond distance in a graphite mono-layer is expected to be somewhat shorter than the bulk value[53].

The total energy of these molecules can be accurately fitted with a two-parameter expression similar to that given in Equation 1:

$$E_{\text{tot,est}} = 6N^2E_C + 6NE_H \quad (2)$$

Table 1 shows that the total energies of the systems studied here are reproduced by Eq. 2 with an error smaller than 0.2 kcal/mol per carbon atom.

The optimum coefficients in Equation 2 are  $E_C = -37.8363$  and  $E_H = -0.5685$  Hartree.  $E_C$  is very close to the value -37.8366 found for the pure graphite clusters.



**Figure 5.** HOMO and LUMO orbital energies for  $C_6N_2H_6N$ , plotted vs  $1/N$ .

The value of  $E_H$  corresponds to a contribution of 47.1 kcal/mol to the total energy of  $C_6N_2H_6N$  for each bonded H-atom (the hydrogen atom has an energy of -0.4935 Hartree in the basis set used).

Alternatively, the parameter values can be interpreted as 83.3 kcal/mol per C-C bond, 88.7 kcal/mol per C-H bond.

The value 125 kcal/mol represents an upper bound to the cohesive energy per carbon atom in graphite, since the interaction between layers in the bulk has not been accounted for. Given the relatively large distance and the physical properties of graphite, the inter-layer interaction energy is estimated to be < 5 kcal/mol.

This leaves us with a computed result in less than satisfactory agreement with the experimental value of about 170 kcal/mol[54]. The neglect of electron correlation and the limited basis set used are the most important sources of the discrepancy. In a previous study on mono-layer graphite[53], basis set effects were found to lead to a significant underestimation of the cohesive energy.

The orbital energies show a surprisingly slow convergence as the size of the molecule increases. Even for the largest system studied, the HOMO-LUMO gap is about 4 eV. From the values shown in Fig. 5 one may expect semiconducting behavior to occur at  $N=8-10$ , i.e. for clusters with 400-600 atoms. At that point a conventional Hartree-Fock approach would of course break down.

The HOMO and LUMO orbital energies seem to converge towards a value of about -4 eV, which would be an estimate of the work function for single-sheet graphite. This is in reasonable agreement with the work function of 4.9 eV experimentally found for bulk graphite[52].

### Diamond-like Clusters.

From the two-dimensional, graphite-like clusters, the extension to three-dimensional structures is obvious. Symmetric structures developed in a similar fashion to the planar systems would grow in three dimensions with increasing  $N$ , and the number of atoms would increase faster. In this work clusters of  $T_d$  symmetry were studied, resembling a small fragment of a diamond structure. Only systems with saturated external bonds were considered. The number of carbon and hydrogen atoms in such a structure is given by

$$N_C = N(4N^2 - 1)/3$$

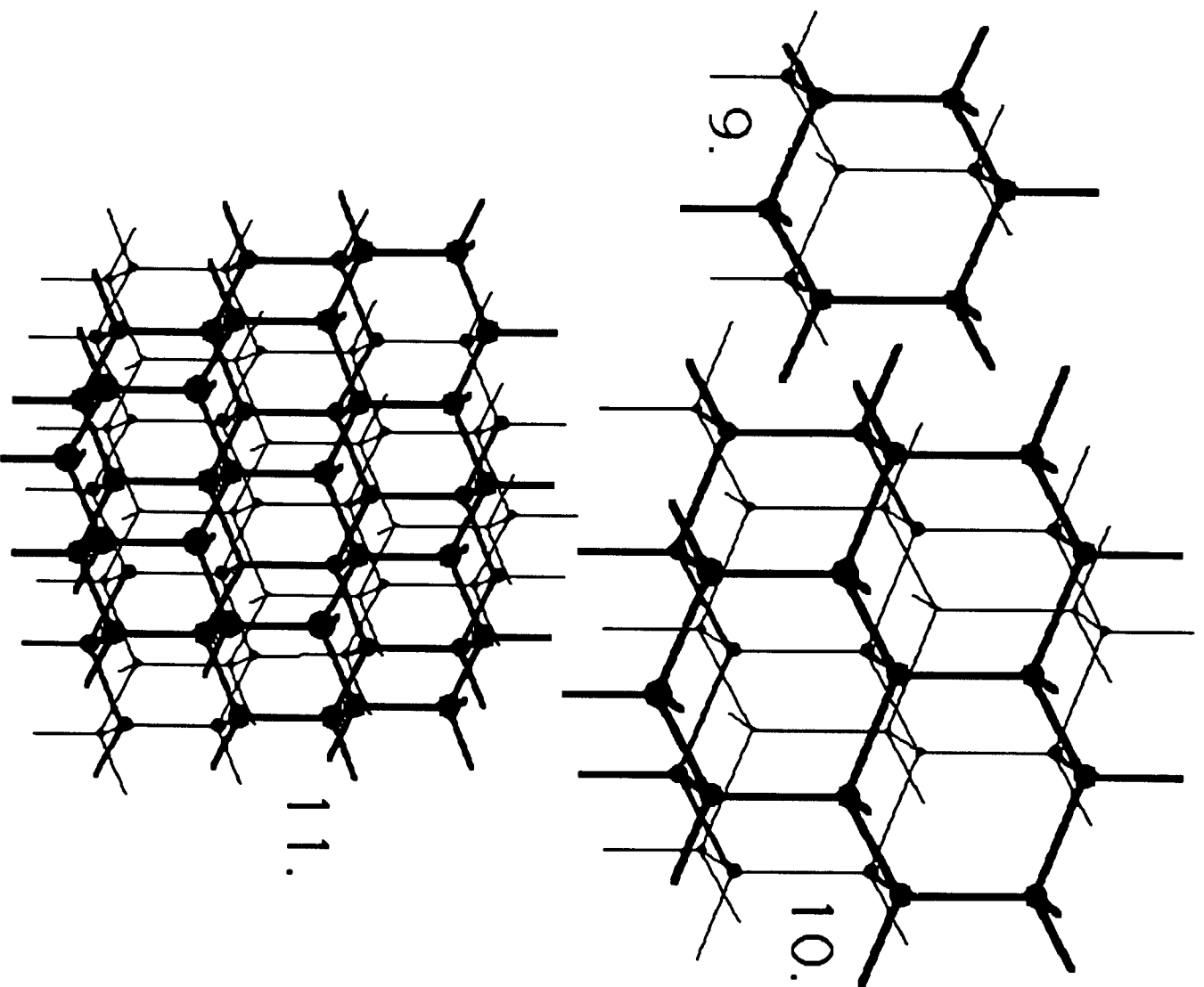
$$N_H = 4N^2$$

Here we present some results from studies on systems with  $N=2,3$ , and 4. ( $N=1$  would correspond to the methane molecule). The molecules are shown in Fig. 6

For all three molecules, an overall C-C distance was optimized. The values obtained for the three systems are 1.542Å, 1.540Å and 1.539Å, smoothly converging to a value slightly shorter than the equilibrium distance in diamond.

Fitting the energies to an expression similar to Eq 2 gives  $E_C = -37.8360$ ,  $E_H = -0.5732$  for the tertiary hydrogens, and  $E_H = -0.5742$  for methylene carbons. The extrapolated cohesive energy is 125 kcal/mol, the same as for graphite. A breakdown of the bond energies per bond gives a C-C bond energy of 62 kcal/mol. The C-H bond energies are 82 and 81 kcal/mol for the methylene and the tertiary hydrogens, respectively.

The convergence pattern for the orbital energies is quite different from that found in the graphite-like clusters as shown in Fig. 7. The extrapolated band gap is somewhat uncertain but seems to lie around 10 eV, and is definitely larger than the experimental value of about 4.6 eV. This difference is mainly due to neglect of electron correlation in our calculations.



**Figure 6.** The diamond-like systems C<sub>10</sub>H<sub>16</sub>(9), C<sub>35</sub>H<sub>36</sub>(10) and C<sub>84</sub>H<sub>64</sub>(11).



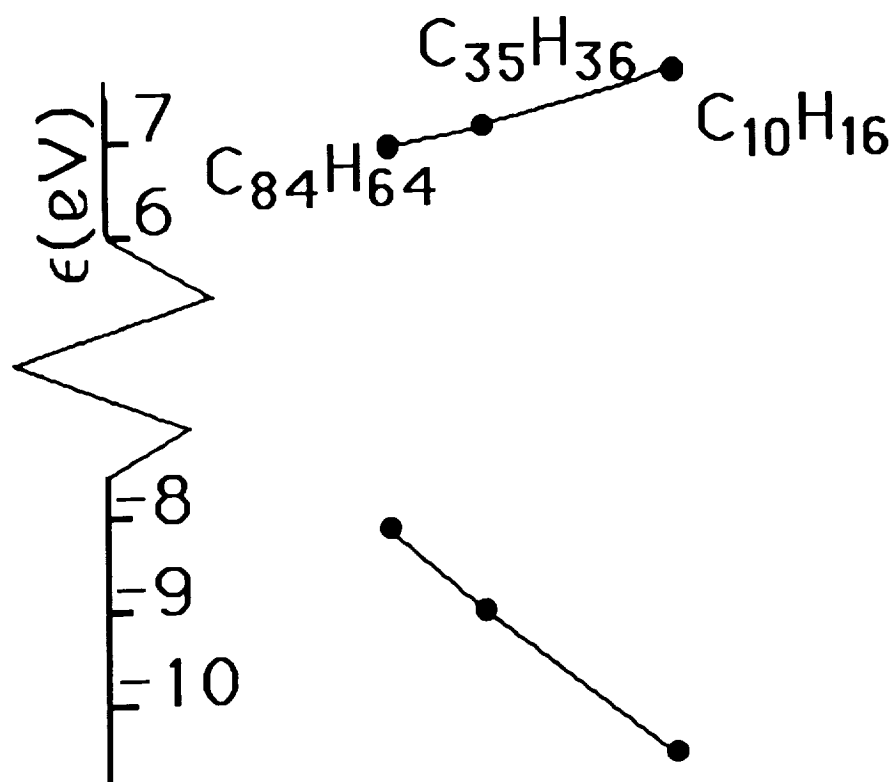


Figure 7. HOMO and LUMO energies for the diamond-like clusters, plotted vs  $1/N$ .

### Linear Carbon Chains.

Another, simple form of elemental carbon would be chains formed from carbon atoms. As a prototype model a single-stranded chain is most suitable. If branching were to be considered, all intermediate forms up to and including the diamond- and graphite-like clusters would be included. For non-branched chains, the two variants to choose from are a system of alternating singly and triply bonded carbon atoms (poly-ynes), and a system with all double bonds (cumulenes). Cumulene structures are assumed to be the preferred ones for odd-membered chains, whereas the even ones may have some poly-yne character. Recent studies on linear  $C_6$  show that a cumulene-like structure is preferred, both at the SCF level and when correlation is accounted for[50].

As an alternative to linear chains, a simple ring-shaped molecule should also be considered. Regardless of whether poly-ynes or cumulenes are considered, the gain in bond energy due to the new bond formed should be relatively independent of the size of the chain. In contrast, the strain involved in forming a ring is inversely proportional to the number of atoms, assuming a harmonic C-C-C bending potential. Clearly, ring structures should be thermodynamically preferred for chains above a certain size (even though their formation might be kinetically or statistically unfavorable). In fact, already for as small a system as  $C_6$  the ground state structure is found to be cyclic, although the omission of electron correlation would predict a linear, cumulene-like geometry to be marginally lower in energy[50].

We have chosen to study the  $C_{20}$  poly-yne ring assuming it to be a reasonable representative for a large chain molecule. The bond lengths optimized at the Hartree-Fock level are 1.37 Å and

1.20 Å, respectively. The same values are found for the experimental bond lengths in 1,3-butadiene  $\text{CH}_3\text{-C}=\text{C}=\text{C-H}$ , indicating that there is very little  $\pi$  conjugation in the system.

The cohesive energy per carbon atom in a poly-yne ring is only 99.1 kcal/mol, clearly lower than the value in e.g. planar  $\text{C}_{54}$ . In addition to the unfavorable energy one would anticipate a long and complicated route of formation for a chain-like molecule when starting from graphite, and it does not seem likely that any of the larger clusters observed experimentally would have a linear or cyclic chain structure.

### Non-planar Clusters Containing Five-membered Rings.

The existence of a stable  $\text{C}_{60}$  molecule, *Buckminsterfullerene* was recently proposed[14]. In the suggested structure, twelve regular pentagons and twenty hexagons are connected to form an almost perfectly spherical pattern of icosahedral symmetry.

Previous theoretical work seems to support the existence of this amazing molecule. Several calculations[25-41] on *Buckminsterfullerene* at various degree of approximation find a resonance stabilization larger than in benzene, and only slightly smaller than in graphite. From these calculations it has been concluded that the molecule is likely to exist. A recent MNDO study[41] concludes that large polyhedral complexes ( $> 40$  atoms) are more stable than the corresponding graphite-like ones. However, the predictive power of these approximate methods is limited, in particular for problems where planar and non-planar systems are compared. The interpretation of the original experiment postulating the existence of *Buckminsterfullerene* has recently been challenged[11], and *ab initio* calculations of the relative energies involved could be used to resolve some of the controversy.

The optimized geometry has twelve regular five-membered rings with an edge of 1.453Å. Each of the thirty hexagons shares three sides with pentagons, whereas the three others, shared with adjacent hexagons, are substantially shorter (1.369Å). Our calculated HOMO-LUMO splittings are around 8 eV, both at the minimal-basis and double-zeta level. The results of our calculations on *Buckminsterfullerene* were reported fully in Ref 39, and are summarized in Table 3.

The ionization potential (7.9 eV) falls right outside the bracket of experimental IP's reported for carbon clusters with 40 to 100 atoms ( $6.42 \text{ eV} \leq \text{IP} \leq 7.87 \text{ eV}$ [11]). Inclusion of correlation effects will lower the calculated  $\Delta\text{SCF}$  IP by 0.25 to 0.50 eV, so that the corrected IP will be at the upper end of the experimental IP-bracket. Due to the diffuseness of the  $\pi$  orbital from which an electron is removed, the correlation error in the  $\Delta\text{SCF}$  value will be smaller than in cases where an electron is removed from a well localized bond. In those cases a correction of 1 eV is usually applied.

The cohesive energy per carbon atom in *Buckminsterfullerene*, 114 kcal/mol, is 11 kcal/mol lower than the value extrapolated for graphite, but 7 kcal/mol higher than the value computed for the  $\text{C}_{54}$  graphite-like sheet or 14.5 kcal/mol higher than for the  $\text{C}_{20}$  poly-acetylene ring. Accordingly, the heat of formation for *Buckminsterfullerene* is 650 kcal/mol, suggesting a high degree of instability with respect to graphite.

At the Hartree-Fock level, comparisons between systems with very different molecular and electronic structures have to be made with some care. Strained geometries of the type found in  $\text{C}_{60}$  are usually difficult to describe without polarization functions. The basis set used is therefore expected to slightly favor the planar systems. Repeating the calculations with d-functions added would be unnecessarily time-consuming, and another approach has instead been used. The bowl-shaped corannulene molecule ( $\text{C}_{20}\text{H}_{10}$ ) has a geometry resembling a fragment of a  $\text{C}_{60}$  ball, and the strain in the C-framework ought to be similar as well.

To investigate the basis set effect in connection with geometric strain in *Buckminsterfullerene*, we have performed calculations with and without d-type functions on corannulene. The d-functions

improve the binding with about 10 kcal/mol per C-atom in  $C_{20}H_{10}$ ; the corresponding improvement in coronene ( $C_{24}H_{12}$ ) is 8 kcal/mol. Within reasonable limits, these numbers are not crucially dependent on the d-exponents used (0.4-0.6). One can therefore estimate that the inclusion of d-orbitals in *Buckminsterfullerene* would decrease the calculated heat of formation by about 120 kcal/mol.

Even though the predicted relative instability of *Buckminsterfullerene* would be somewhat diminished by such an extension of the basis, the main conclusion remains; the  $C_{60}$  molecule is still about 530 kcal/mol higher in energy than a corresponding fragment of bulk graphite.

Another conclusion that can be drawn from the calculations on corannulene is an estimate of the loss of energy due to incorporation of a five-membered ring into a structure of condensed six-rings. Eq. (2) predicts a total energy of -762.4110 Hartree. for  $C_{20}H_{10}$ , the energy actually computed is -762.2656 Hartree., and the loss due to a five-membered ring is thus about 0.14 Hartree. This is significantly larger than loss of 0.09 Hartree. predicted from Eq. (1) due to the occurrence of a dangling bond in the structure. It can therefore be concluded that the reducing the number of dangling bonds in 2 and 3 above by introducing five-membered rings on the periphery is not likely to lead to more stable structures.

In conclusion, these calculations suggest that the *Buckminsterfullerene* molecule is thermodynamically unstable with respect to graphite by about 23 eV. In general, thermodynamically unstable molecules can often be readily synthesized, and frequently exist with virtually infinite lifetimes. The unusually large instability observed in this case might seem almost prohibitive, however no other good candidate for the pronounced peak seen at  $n=60$  in the reported mass spectra has been found. Apparently, the bond strain in *Buckminsterfullerene* is still more favorable than a situation with 20 unpaired electrons. Multiple-sheet models have not been considered in this work, since the number of dangling bonds in these would be even larger.

### Conclusions.

We have demonstrated that new and unique information about large molecular systems can be achieved by using computational methods on a large scale. In many cases, that information would have been very difficult to obtain with other means.

Even though our calculations on PAHs show a fairly slow convergence of properties, they allow for an extrapolation on the cohesive energy per carbon atom in bulk graphite. The data obtained from the Mulliken population analysis further show that the inner parts of the larger molecules studied have a domain with little total charge or spin density, which may mimic a graphite surface rather well. Since the problem of dealing with a large number of open shells can be circumvented by these calculations, the approach offers an attractive way of modeling a graphite surface as well as a way to study graphite intercalation compounds.

The fact that pairing up dangling bond electrons may lead to more stable graphite fragments is somewhat surprising. This suggests that the edge of a graphite fragment may look different from what is commonly assumed. This observation may have far-reaching consequences for the understanding of the chemistry and reactivity of large carbon clusters.

Energetically, the lively debated soccerball-form of  $C_{60}$  compares very favorably with a graphite-like sheet of carbon atoms. This, of course, does not prove that *Buckminsterfullerene* really is (fully or partly) responsible for the  $C_{60}$  peak observed. Due to the large number of degrees of freedom, a study of all plausible isomers would be a prohibitively cumbersome task. Even if such a complete coverage were possible the existence of different molecular species at these conditions is not likely to be governed by thermodynamic stabilities only.

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Table 1: Total energies and C-C bond distances computed for  $C_{6n}2H_{6n}$  and energies estimated using expression (2) with the parameters  $E_C=-37.8363$ ,  $E_H=-0.5685$  Hartree. The C-H distances were kept fixed at 1.10Å.

n	system	$-E_{tot,calc}$	$-E_{tot,pred}$	$\Delta$	$R_{cc}$ (Å)
1	$C_6H_6$	230.4320	230.4288	0.0032	1.384
2	$C_{24}H_{12}$	914.8938	914.8932	0.0006	1.401
3	$C_{54}H_{18}$	2053.3942	2053.3932	0.0010	1.404
4	$C_{94}H_{24}$	3645.9003	3645.9288	-0.0285	1.406
5	$C_{150}H_{30}$	5692.4981	5692.5000	-0.0019	1.406 <sup>a</sup>

<sup>a</sup>assumed without geometry optimization.

**Table 2: Total computed energies and distances for the diamond-like clusters.**  
**The C-H distances were kept fixed at 1.09Å.**

n	system	-E <sub>tot</sub> (a.u.)	R <sub>cc</sub> (Å)
2	C <sub>10</sub> H <sub>16</sub>	387.54332	1.542
3	C <sub>35</sub> H <sub>36</sub>	1344.90665	1.540
4	C <sub>84</sub> H <sub>64</sub>	3214.91903	1.539

**Table 3: Computed properties for *Buckminsterfullerene*.**

**Bond lengths:**

R1 1.453 Å

R2 1.369 Å

**Ionization potential:**

ΔSCF 7.92 eV

HOMO energy 8.24 eV

**Electron affinity:**

ΔSCF 0.80 eV

LUMO energy 0.60 eV

**Cohesive energy/carbon atom:** 114 kcal/mol